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Dynamic toxicity modelling based on the USEtox matrix framework

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scenario system, monitoring studies were conducted at the scenario sites during past years. Comparison of the 90th percentile of maximum daily predicted exposure concentrations (PECs) with the maximum measured concentrations of local used pesticides revealed acceptable agreement for rice-surface water scenarios, but for row crop-surface water and ground water scenarios, more filed monitoring data are required for adequate validation.

117 Conduct of a Groundwater Monitoring Study using Statistically Valid Survey Approaches to Contextualise PECGW Estimates Obtained from Regulatory Models D. Wallace, Environmental Safety Environmental Fate; P. Sam, Syngenta Ltd / Environmental Safety Environmental Fate; P. Hendley, Phasera Ltd; A. Newcombe, ARCADIS US Inc. Current regulations governing the registration of plant protection products in the European Union (1107/2009) mandate that an assessment for the potential to reach groundwater is made, primarily using models such as PEARL and PELMO. However, monitoring programs allow the opportunity to measure real-world distributions of concentrations in shallow groundwater to help put the modelled estimates into context. An extensive pan-European groundwater monitoring study was initiated in 2012 to investigate and quantify the distribution of concentrations of two metabolites in very shallow groundwater beneath fields with a history of at least 3 years of herbicide use in the previous 5 years. In order to permit the extrapolation of study findings to all settings where the herbicide is used in EU, the study was designed to ensure selected sites would be spatially distributed to reflect a wide range of agronomic and climatic settings and that the site search would be focused in areas with larger amounts of maize agriculture, higher probabilities of the occurrence of shallow groundwater and in areas where the climatic conditions were favourable for higher metabolite leaching if the herbicide were applied. FOCUS groundwater modelling was conducted to examine the potential for the metabolites to leach following application to maize. The FOCUS simulation models FOCUS-PEARL (v 4.4.4) and FOCUS-PELMO (v 5.5.3) were used in the modelling study. This data is compared with the analytical data generated from groundwater samples collected from installed monitoring wells between March 2013 and July 2014. It was found that at 90% of these very vulnerable sites with a prolonged history of herbicide use and very shallow groundwater, the ground water sampled just downstream of the treated plots contained < 7.6 µg/L of metabolite A and In conclusion, careful monitoring studies designed to follow statistically valid survey sampling approaches can provide solid science based data to put model predictions into context. This study shows clearly that current regulatory modeling for polar metabolites produces PECGW estimates that greatly over-estimate real world concentrations.

118 Pesticide exposure modelling in drinking water supply catchments: opportunities, challenges and uncertainties S. Pullan, TSGE Consulting; M. Whelan, University of leicester / Geography; I. Holman, Cranfield University / Energy Environment and Agrifood. Pesticides continue to challenge Drinking Water Directive compliance in many surface water catchments used for drinking water supplies in Europe, most commonly due to diffuse-source inputs from agriculture. Catchment-scale modelling is a useful tool for assessing non-compliance risks in such catchments, for helping to identify and prioritise catchment-specific monitoring strategies and for helping to target potential catchment management interventions (e.g. restricted pesticide use on high risk soils). Although models are used for pesticide risk assessment in the EU regulatory authorisation process, these models employ standardised field-scale scenarios which do not necessarily reflect the spatial complexity of the agricultural landscape or temporal complexity of the catchment hydrological response. Small-catchment scale modelling has been identified by the FOCUS Landscape and Mitigation group as a possible higher-tier refinement to FOCUS Step 3 modelling. A simple process-based water balance model linked with a pesticide fate and transport model is described in this presentation. The model predicts daily discharge and chemical concentrations at the catchment scale for a given land use distribution and pesticide application pattern. Physical parameters were derived from the UK soil properties database. The model has been calibrated and validated successfully in five UK catchments for nine pesticide active ingredients. The challenges, uncertainties and opportunities of catchment-scale modelling during model development and model application are discussed.

119 Occupational exposures to chemical in Life Cycle Assessment G. Kijko, CIRAIG - École Polytechnique de Montréal / Génie Industriel; O. Jolliet, University of Michigan / Environmental Health Sciences School of Public Health; M. Margni, Ecole Polytechnique de Montreal / Mathematical and Industrial engineering. Life Cycle Assessment (LCA) is a comparative method that aims to assess potential environmental impacts of a product life-cycle onto several “protection areas”. It helps preventing burden shifts from one area to another while minimizing the global life-cycle . Human Health is one of these areas covered by LCA and notably include potential impacts on Human Health from exposures to chemicals emitted to the outdoor environment by industrial processes and activities along the product life cycle. However, indoor exposure of workers have not yet been included in the LCA framework despite its known contribution to occupational impacts. This research aims to (a) developp a novel methodology linking measured occupational concentrations to potential impacts to workers within the LCA framework, (b) expand this approach to adress occupational exposure across the whole product supply chain and (c) apply these methods to a case study identify hotspots in the life-cycle and to compare the occupational exposures to population exposures due to outdoor emissions. This research shows that potential impacts due to occupational exposures to chemicals are not negligible when compared to other well known source of impacts on Human Health. We show that potential impact for the whole industrial sectors during one year is equivalent to the annual impacts from PM 2.5 exposures due to outdoor emissions. We also demonstrate that depending on the industrial sector the main contributor to the occupational exposures may be found along the supply chain rather than the industry itself: the relative contribution of the supply chain to the total potential impact on worker ranges from 10% up to more than 85%. and should therefore be included in the scope of Life Cycle Assessment. This research shows the relevance to include occupational exposure in LCA and provides an operational method allowing practitioners to include it in LCA studies. We provide direct, indirect (supply chain) generic characterization factors for occupational exposures in each industrial sectors. This enables practitioners to integrate occupational exposures to chemical in LCA. The method allos the use of more specific data (concentrations, hours) when it is available.

120 Dynamic toxicity modelling based on the USEtox matrix framework P. Fantke, Technical University of Denmark / Quantitative Sustainability Assessment; O. Jolliet, University of Michigan / Environmental Health Sciences School of Public Health; C. Wannaz, The Unversity of Michigan, Ann Arbor / SPHEHS. While it is recommended to report characterization factors for different time horizons, e.g. for infinity (steady-state) and after 100 years, the UNEP/SETAC toxicity model USEtox 1.01 only allows for steady-state calculations. The present paper addresses this lack of temporal flexibility and aims to a) develop a dynamic multimedia model based on and fully compatible with the USEtox steady-state matrix framework, b) analyze and interpret the main parameters affecting chemical fate and exposure dynamics, and c) evaluate whether for 3000+ USEtox 1.01 chemicals a 100 years time horizon will yield considerably different results than the steady-state default assumption. To solve the dynamics of the system, we apply a classical approach based on Eigenvectors and Eigenvalues that diagonalizes the rate constants matrix. The fate factor matrix after 100 years can then be calculated as a simple matrix equation as a function of Eigenvectors Eigenvalues. Results show that for organic compounds, such as dioxin, masses in all compartments saturate (i.e. reach steady-state) within 100 days, whereas for metals, such as lead, the soil and deep ocean compartments are far from steady-state even after 100 years. The Eigenvectors and Eigenvalues also help interpreting and understanding the kinetics in each compartment. For the 3000+ organic compounds in USEtox 1.01, there is no difference in fate factors or subsequent intake fractions between 100 years and steady-state values. The only difference appears for metals fate in the deep ocean and in soil, with a reduction of both fate factor in soil and related intake of agricultural produce after 100 years to between 7% and 84% of the steady-state values. We conclude that considering a time horizon for metals of 100 years raises the question of the consistency between LCIA results and LCI emissions from metals deposited in landfills, which can span several 1000 years.

121 Validation of the results from toxicity assessment in LCA using triangulation S. Roos, Swerea IVF AB / Chemical Engineering; G. Peters, Chalmers tekniska högskola. The European Commission initiative for Product Environmental Footprint is based on life cycle assessment (LCA), with the USEtox consensus model as the recommended impact assessment method for toxicity. The confidence in the scientific robustness will be crucial for the intended users to take actions based on the results. This research work aims to validate the results from toxicity assessment within the context of LCA by benchmarking USEtox with two alternative approaches in a case study. While strictly speaking there can be no experimental validation of environmental damage predicted in an LCA of a generic product, comparison of the results of three different methods can be considered a form of triangulation in LCA which can potentially provide confidence in an individual method. A textile case was chosen as the textile industry is an intense user of chemicals.Three different quantitative or semi-quantitative methods for toxicity assessment were used: the USEtox model chosen for the European PEF work; the Score System presented in the European Commission's Reference Document on Best Available Techniques for the Textiles Industry; and the Strategy Tool presented by Askham. The results show that the three methods do not give a consistent toxicity assessment of the chemicals in the case study. For USEtox the result also depends on whether the practitioner uses the default method or add more characterization factors. The two semi-quantitative methods give more equal importance to the chemicals while the USEtox scores differ by several orders of magnitude. The Simple Score System and the Strategy Tool are very concerned with persistent pollutants and therefore the chemicals which are not readily biodegradable, receive a high score. The USEtox score on the other hand is relatively low for the persistent organic chemicals. Validation of results using triangulation can be used both to create confidence and/or help identify new challenges that were not previously perceived in the method. In this case we showed that the property of persistence is judged to have lower importance in USEtox compared to the two other methods, which is a finding that can be used to develop the fate modelling in USEtox. On the other hand, USEtox could provide additional advice compared to the two other methods, that one of the substances could be more environmentally problematic than what these semi-quantitative methods signals.

122 Approach for a Human and Eco Toxicity Indicator for Construction Products and Works (ToxScale)P. Saling, BASF SE / Sustainability Strategy; F. Kalberlah, FoBiG GmbH; Q. de Hults, BASF SE; B. Grahl, Fa. Integrahl; E. Schmincke, PE-International. Currently, potential toxicological and eco-toxicological impacts of construction products and works are insufficiently characterised. There are no meaningful indicator(s) for a comparative ranking to assist declaration, selection and substitution decisions. At least at present, characterisation models like USEtox have serious limitations to adequately describe potential toxicological and eco-toxicological impacts for a complex life cycle of construction products with heterogeneous exposure conditions from cradle to grave. One reason is the very limited availability of qualified data. However, substance information generated within REACH registration could provide a wealth of useful data to describe health and eco-toxicological impact. Because of the different philosophies of REACH and LCIA characterisation models, it may be difficult to directly make appropriate use of REACH data within LCIA. Therefore, an indicator is proposed, which is applicable in Environmental Product Declarations (EPD) providing additional human health and eco information to LCIA according to ISO 14025. This indicator, “ToxScale”, uses REACH information for toxicological and eco-toxicological characterisation of construction products. This paper provides an outline of the ToxScale approach. At this stage, discussion is restricted to human health impact, but may be extended to eco-toxicity. ToxScale is characterised with: 1) a hazard score based on “derived no effect level” (DNEL) 2) an exposure modifier related to the REACH “risk characterisation factor” (RCR), 3) REACH specific descriptors for environmental release categories (ERCs) and process categories (PROCs) to quantify emissions with potential impacts for all stages of a substances’ life cycle, 4) an aggregation procedure aggregating along different life cycle stages, and 5) a supplemental procedure to address substances, exposure scenarios, life cycle stages and inherent toxicity, which are not adequately addressed under REACH, but may contribute to the potential impact of a construction product. ToxScale integrates REACH thinking and LCIA thinking as well as “risk” and “hazard” thinking to build an indicator, which permits construction products’ ranking based on potential health and eco-toxicological impacts as a supplement to LCIA.

123 A strategy to deal with information of differing quality exemplified by the use of QSARs to fill the algae data gap in an LCIA of plastic additives J.E. Grönholdt Palm, Department of Studies in Environmental Science; T.V. Rydberg, M. Rahmberg, IVL Swedish Environmental Research Institute; H. Andersson, IVL Swedish Environmental Research Institute Ltd / Department of Chemical and Biological Engineering; U. Sahlin, Linnaeus University, School of Natural Sciences. Data gaps are problematic when screening for dangerous substances or in impact assessments where several chemicals are considered for evaluation. Lacking testing information can be replaced by non-testing information such as Quantitative Structure Activity Relationships (QSARs), but even though this latter information comes with lower reliability, this is seldom taken into account in the forthcoming assessments. The difficulty to meet standards for best information calls for strategies to handle data gaps which take varying reliability in information into account. Using safety factors when reliability is low can be problematic since this result in more conservative evaluations of substances for which information is of low reliability and an unknown level of risk aversion in the assessment. An alternative is to reflect lower reliability using probability distributions representing the expected error in the information and propagate this uncertainty in the forthcoming assessments using Monte Carlo analysis. It is even possible to let the error to expect from QSARs depend to what extent a substance falls inside the models domain of applicability. QSARs cannot fill all gaps in data. Default values can be used instead of leaving substances out of assessments, but if so, these should reflect low reliability as well. We demonstrate the practical implications of four strategies to handle varying reliability in information on algal toxicity in a Life Cycle Impact Assessment on 159 plastic additives of concern using emissions from societal plastic materials in Sweden. A review concluded that a small amount of these substances had toxicity data for algae *Pseudokirchneriella subcapitata*. A QSAR was constructed which provided non-testing algal information of substances inside and on the border of the models domain of applicability evaluated by PmodXPS. Substances with neither testing nor non-testing information were assigned default values. Screening based on characterization factors resulted in different rankings of substances when changing the level of cautiousness. The different strategies to handle varying reliability in information do more or less open up for quantifying uncertainty in Life Cycle Impact Assessments.

124 Consensus building results on the new scarcity indicator from WULCA A. Boulay, CIRAIG - École Polytechnique de Montréal / Chemical engineering department; J.C. Bare, US EPA / National Risk Management Research Laboratory; L. Benini, JRC Institute for Environment and Sustainability - European Commission / Sustainability Assessment unit; M. Berger, Technische Universitaet Berlin / Chair of Sustaiable Engineering Office Z; C. Bulle, CIRAIG - ESG - UQAM / Strategy corporate social responsibility; I. Klemmayer, Institute for Water Resources and Water Supply; M. Lathuilliere, University of